Supplementary material

Table S14 – Summary information about findings of our study, including the comparison with reference values reported by Trabado et al. 2017 (Trabado et al., 2017), the percentage of variation identified in the Tobit models, and a comparison with other studies.

Chemical characteristic	Differences with Trabado et al. 2017	Tobit (Δ%)	Studies which found similar associations	Studies with findings in disagreements with ours
Amino acids positively associated with BMI				
Valine (BCAA)	our results> reference values	+23.2	(Bagheri et al., 2019, 2018; Cirulli et al., 2019; Dunn et al., 2015; Ho et al., 2016; Kim et al., 2010; Libert et al., 2018; Newgard et al., 2009; Wang et al., 2018; Xie et al., 2014)	
Isoleucine (BCAA)		+20.0		
Leucine (BCAA)	our results> reference values	+15.0		
Tyrosine (aromatic aa)	our results>> reference values	+29.8	(Cirulli et al., 2019; Dunn et al., 2015; Ho et al., 2016; Libert et al., 2018; Rangel-Huerta et al., 2019; Wang et al., 2018)	
Phenylalanine (aromatic aa)	our results>> reference values	+20.4		
Tryptophan (aromatic aa)				It was higher in (Kim et al., 2010; Wang et al., 2018; Yu et al., 2018)
Alanine (hydrophobic aa)	our results> reference values	+18.9	(Bagheri et al., 2019; Dunn et al., 2015; Ho et al., 2016; Libert et al., 2018)	
Proline (hydrophobic aa)		+18.1	(Bagheri et al., 2019; Dunn et al., 2015)	
glutamic acid (negative polar aa)	our results>> reference values	+17.1	(Bagheri et al., 2019, 2018; Carayol et al., 2017; Wang et al., 2018; Zhao et al., 2016)	
Lysine (positive polar aa)	our results> reference values	+7.1	(Dunn et al., 2015; Libert et al., 2018)	
Ornithine (positive polar aa)	our results>> reference values	+9.2	(Dunn et al., 2015)	
Amino acids negatively associated with BMI				

Asparagine (uncharged polar aa)	reference values>our results	-16.1	(Bagheri et al., 2019; Dunn et al., 2015)	
Glycine (uncharged polar aa)		-13.6		It was higer in (Oberbach et al., 2011)
Histidine (Charged polar aa)		-11.8		
Serine (Uncharged polar aa)		-10.0	(Bagheri et al., 2019; Dunn et al., 2015)	
Citidine (polar aa)		-6.2		It was not significative in (Dunn et al., 2015)
Threonine (Uncharged polar aa)				It was not significative in (Dunn et al., 2015)
Arginine (Positive polar aa)	reference values>>our results			
Biogenic amines positively associated with BMI				
Kynurenine	our results>> reference values	+16.1	(Carayol et al., 2017; Ho et al., 2016; Zhao et al., 2016)	
Aminoadipic acid		+18.5		
4-hydroxyproline		+8.0		
Biogenic amines negatively associated with BMI				
Serotonin		-7.4		
Creatinine	reference values>our results	-6.1		Higher in (Dunn et al., 2015)
N-acetylornithine		-9.2		
Acylcarnitines positively associated with BMI				
C0		+12.6	(Cirulli et al., 2019; Xie et al., 2014)	Lower in (Kim et al., 2010)
C3		+12.2	(Cirulli et al., 2019; Kim et al., 2010; Libert et al., 2018; Xie et al., 2014)	
C2		+9.1		

C5				
C18.1	our results> reference values	+5.7 (FDR P=0.070)		
Acylcarnitines negatively associated with BMI				
C12		24.5		
LysoPC positively associated with BMI				
lysoPC a C16:1		+7.3	(Bagheri et al., 2019)	
LysoPC negatively associated with BMI				
lysoPC a C26:0	reference values>>our results			
lysoPC a C28:0	reference values>>our results			
lysoPC a C18:2	reference values>our results	-23.3	(Bagheri et al., 2019, 2018; Carayol et al., 2017; Ho et al., 2016; Tulipani et al., 2016; Wang et al., 2018)	
lysoPC a C28:1	reference values>our results			
lysoPC a C18:1		-15.9	(Bagheri et al., 2019, 2018; Carayol et al., 2017; Ho et al., 2016; Kim et al., 2010; Tulipani et al., 2016; Wang et al., 2018)	
lysoPC a C17:0		-14.3	(Tulipani et al., 2016)	
PC aa positively associated with BMI				
PC aa C38:3	our results>reference values	+21.1	(Bagheri et al., 2019, 2018; Carayol et al., 2017; Ho et al., 2016)	
PC aa C40:4		+14.3		
PC aa C32:1		+12.4	(Bagheri et al., 2019, 2018; Carayol et al., 2017)	(Oberbach et al., 2011)
PC aa C38:4		+7.6	(Carayol et al., 2017)	
PC aa C40:5		+6.9		(Oberbach et al., 2011)
PC aa negatively associated with BMI				
PC aa C38:6	reference values>>our results	-12.9	(Ho et al., 2016)	
PC aa C38:0	reference values>>our results	-11.7		

PC aa C36:0	reference values>our results	-11.7		
PC aa C42:5	reference values>>our results	-11.6		
PC aa C36:6	reference values>>our results	-10.6		
PC aa C34:2	reference values>>>our results	-10.5		
PC aa C42:1	reference values>>>our results	-10.0	(Carayol et al., 2017)	
PC aa C42:6	reference values>>our results	-10.5		
PC aa C40:3	reference values>>our results	-8.8		
PC aa C42:2	reference values>>our results	-9.6	(Carayol et al., 2017)	
PC aa C42:0	reference values>>>our results	-8.4	(Carayol et al., 2017)	Higher in (Oberbach et al., 2011)
PC aa C40:2	reference values>>our results	-7.3		
PC aa C28:1				
PC ae negatively associated with BMI				
PC ae C36:2	reference values>>our results	-20.5		
PC ae C34:3	reference values>>our results	-20.2	(Bagheri et al., 2019)	
PC ae C34:2	reference values>>our results	-18.2		
PC ae C40:6	reference values>>our results	-16.1	(Bagheri et al., 2019)	
PC ae C40:1	reference values>>our results	-16.0		
PC ae C38:0	reference values>>our results	-15.2		

PC ae C36:3	reference values>>our results	-12.3		
PC ae C42:3	reference values>>our results	-11.9	(Carayol et al., 2017)	
PC ae C36:1	reference values>>our results	-10.6		
PC ae C30:0	reference values>>our results	-10.6		
PC ae C40:5	reference values>>our results	-10.5	(Carayol et al., 2017)	
PC ae C42:2	reference values>>our results	-10.1		
PC ae C44:6	reference values>>our results	-10.3	(Carayol et al., 2017)	
PC ae C34:1	reference values>>our results	-9.5		
PC ae C38:6	reference values>>our results	-9.4		
PC ae C32:1	reference values>>our results	-9.0		
PC ae C42:1	reference values>>our results	-8.9		
PC ae C38:5	reference values>>our results	-8.5		
PC ae C42:4	reference values>>our results	-8.4	(Carayol et al., 2017)	
PC ae C34:0	reference values>>our results	-7.8		
PC ae C36:5	reference values>>our results	-7.9		
PC ae C44:5	reference values>>our results	-7.8	(Carayol et al., 2017)	
PC ae C42:5	reference values>>our results	-7.2	(Carayol et al., 2017)	

PC ae C36:0	reference values>>our results	-7.1		
PC ae C32:2	reference values>>our results	-6.7		
PC ae C38:4	reference values>>our results	-6.9	(Bagheri et al., 2019)	
PC ae C38:2	reference values>>our results	-6.1	(Carayol et al., 2017)	
SM positively associated with BMI				
SM C18:1	our results> reference values	8.3	(Ho et al., 2016)	
SM C16:1		7.0	(Ho et al., 2016)	
SM C18:0	our results> reference values		(Carayol et al., 2017; Ho et al., 2016)	
SM negatively associated with BMI				
SM C24:1		-10.5		
SM C16:0		-9.7		
SM C26:1	reference values>>our results	-8.9		
SM (OH) C22:2		-8.3		
SM (OH) C16:1		-6.7		
SM (OH) C14:1		-5.9		
SM C26:0	reference values>>our results			

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